

chain nodes :

14 16

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

12-14 13-16

ring bonds :

1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 5-11 6-13 7-8 8-9 9-10 11-12 12-13

exact/norm bonds :

2-7 3-10 5-11 6-13 7-8 8-9 9-10 11-12 12-13 12-14

exact bonds :

13-16

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:C,H,O

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom  
13:Atom 14:CLASS 16:CLASS

L4 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 2004:203786 CAPLUS  
 DN 140:243724  
 ED Entered STN: 14 Mar 2004  
 TI Cyclopenta[b]naphthalene derivatives  
 IN Lietzau, Lars; Bremer, Matthias; Klasen-Memmer, Melanie; Heckmeier, Michael  
 PA Merck Patent G.m.b.H., Germany  
 SO PCT Int. Appl., 103 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA German  
 IC ICM C07C025-22  
 ICS C07C022-08; C07C025-24; C07C043-225; C09K019-32  
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)  
 Section cross-reference(s): 75  
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004020375	A1	20040311	WO 2003-EP8285	20030728
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	DE 10324843	A1	20041223	DE 2003-10324843	20030602
	AU 2003258538	A1	20040319	AU 2003-258538	20030728
	EP 1532090	A1	20050525	EP 2003-790821	20030728
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	JP 2005537334	T	20051208	JP 2004-569707	20030728
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	DE 2003-10324843	A	20030602		
	WO 2003-EP8285	W	20030728		
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	PATENT NO.	CLASS			
	WO 2004020375	ICM	C07C025-22		
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		IPCR	G02F0001-139 [I, A]; C07C0017-00 [I, C*]; C07C0017-093 [I, A]; C07C0017-25 [I, A]; C07C0017-35 [I, A]; C07C0017-354 [I, A]; C07C0022-00 [I, C*]; C07C0022-08 [I, A]; C07C0025-00 [I, C*]; C07C0025-22 [I, A]; C07C0025-24 [I, A]; C07C0045-00 [I, C*]; C07C0045-46 [I, A]; C07C0045-64 [I, A]; C07C0049-00 [I, C*]; C07C0049-697 [I, A]; C07C0255-00 [I, C*]; C07C0255-52 [I, A]; C09K0019-32 [I, C*]; C09K0019-32 [I, A]; C09K0019-34 [I, C*]; C09K0019-34 [I, A]; C09K0019-54 [I, C*]; C09K0019-54 [I, A]; G02F0001-13 [I, C*]; G02F0001-13 [I, A]		
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		C07C022/08; C07C025/22; C07C025/24; C07C045/46+49/697; C07C045/46+49/755; C07C045/64+49/747; C07C049/697; C07C255/52; C09K019/32; C09K019/34A
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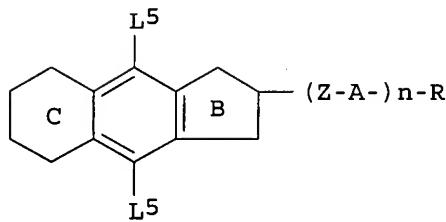
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FTERM 2H088/JA10; 2H088/KA27; 4H006/AA01; 4H006/AA03;  
 4H006/AB64; 4H027/BC05; 4H027/BD10; 4H027/BD11;  
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 4H027/DM05

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NCL 428/001.100; 252/299.610; 252/299.620; 585/021.000  
 ECLA C07C017/093+25/22; C07C017/25+25/22; C07C017/25+25/24;  
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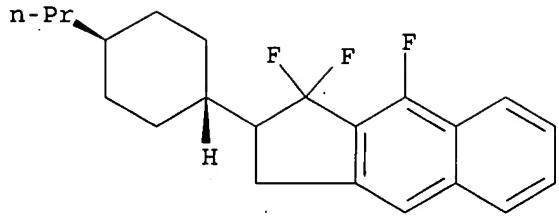
OS MARPAT 140:243724  
 GI



AB The invention relates to cyclopenta[b]naphthalene derivs. of general formula I (C = 6-membered ring with substituents selected from H, C1-15-alkyl, alkoxy, etc.; B = 5-membered ring with substituents selected from H, C1-15-alkyl, alkoxy, etc.; Z = single bond, double bond, -CF2O-, -OCF2-, etc.; A = 1,4-phenylene, 1,4-cyclohexylene, etc.; R = H, C1-15-alkyl, alkoxy, etc.; L5, L6 = H, C1-15-alkyl, alkoxy, etc.; n = 0-3), the use thereof in liquid crystal or mesogenous media, liquid crystal or mesogenous media comprising at least one of said cyclopenta[b]naphthalene

derivs. and electrooptical display elements comprising said liquid crystal  
 or mesogenous media.  
 ST cyclopenta naphthalene synthesis liq crystal mesogenous media  
 electrooptical display  
 IT Liquid crystal displays  
 Liquid crystals  
     (preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal  
     display)  
 IT 666732-85-0P 666732-87-2P 666732-89-4P  
     666732-91-8P 666732-93-0P 666732-95-2P 666732-97-4P  
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     engineered material use); PREP (Preparation); USES (Uses)  
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     7719-09-7, Thionylchloride 57848-46-1 64248-58-4 104089-16-9  
     107263-95-6, N-Fluoropyridinium triflate 610312-65-7 669005-29-2  
     669005-36-1  
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     (preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal  
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     (preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal  
     display)  
 IT 669005-40-7P  
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     use); PREP (Preparation); USES (Uses)  
     (preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal  
     display)  
 RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 RE  
 (1) Clariant International; EP 1223209 A 2002 CAPLUS  
 (2) Hoechst Ag; DE 4434974 A 1996 CAPLUS  
 (3) Merck Patent Gmbh; WO 0246330 A 2002 CAPLUS  
 (4) Montell Technology Co; WO 9846547 A 1998 CAPLUS  
 (5) Yokokoji, O; JP 06263663 A 1994 CAPLUS  
 IT 666732-85-0P 666732-87-2P 666732-89-4P  
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     RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or  
     engineered material use); PREP (Preparation); USES (Uses)  
     (preparation of cyclopenta[b]naphthalene derivs. suitable for liquid crystal  
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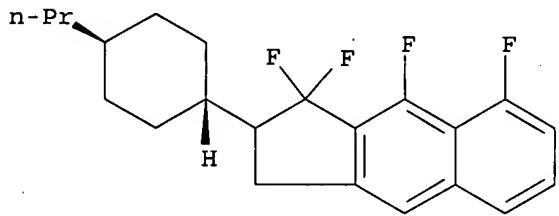
Relative stereochemistry.



RN 666732-87-2 CAPLUS

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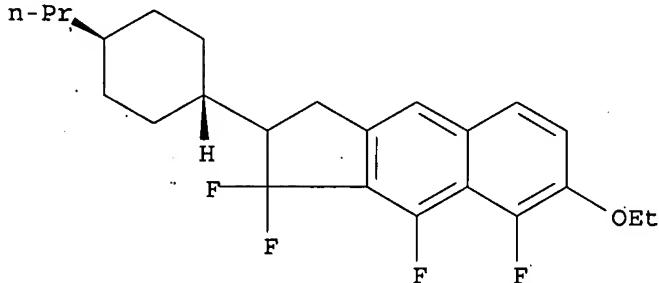
Relative stereochemistry.



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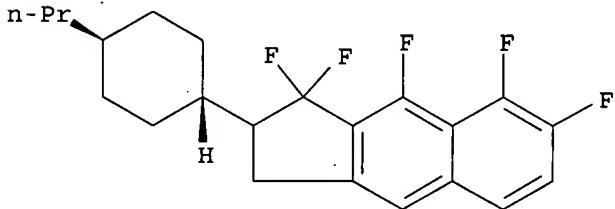
Relative stereochemistry.



RN 666732-91-8 CAPLUS

CN 1H-Benz[f]indene, 1,1,7,8,9-pentafluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

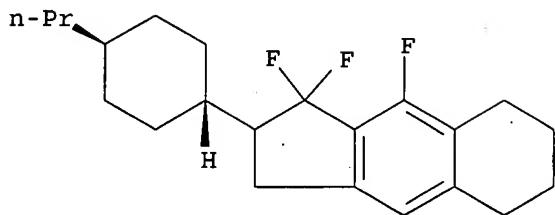
Relative stereochemistry.



RN 666733-11-5 CAPLUS

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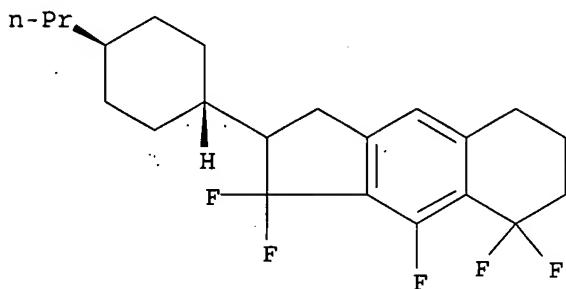
Relative stereochemistry.



RN 666733-13-7 CAPLUS

CN 1H-Benz[f]indene, 1,1,8,8,9-pentafluoro-2,3,5,6,7,8-hexahydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

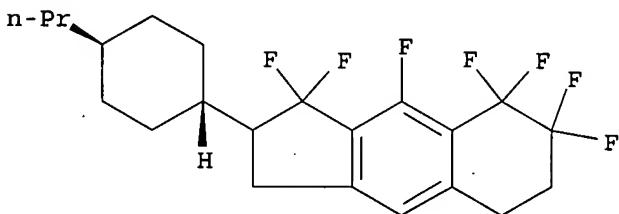
Relative stereochemistry.



RN 666733-15-9 CAPLUS

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Relative stereochemistry.



L4 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:177941 CAPLUS

DN 140:225895

ED Entered STN: 04 Mar 2004

TI Cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display

IN Lietzau, Lars; Bremer, Matthias; Klasen-Memmer, Melanie

PA Merck Patent G.m.b.H., Germany

SO Ger. Offen., 46 pp.

CODEN: GWXXBX

DT Patent

LA German

IC ICM C07C025-22

ICS C07C043-225; C07C049-697; C07D319-06; C09K019-32; C09K019-34;  
G02F001-137; G09F009-35; C07C069-00; C07C323-00; C07C255-00;  
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CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other

Reprographic Processes)  
Section cross-reference(s) : 75

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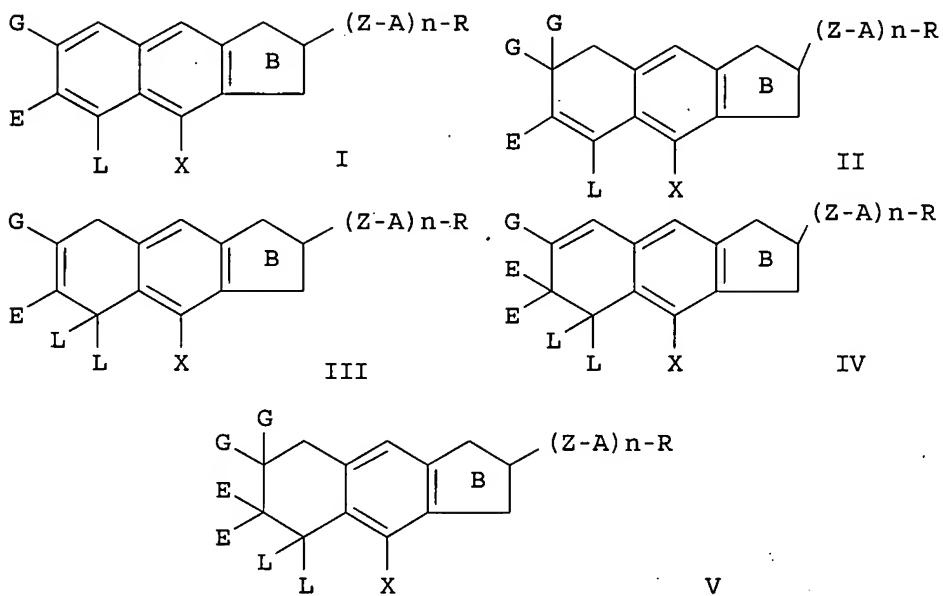
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PI	DE 10238999	A1	20040304	DE 2002-10238999	20020826
	WO 2004020375	A1	20040311	WO 2003-EP8285	20030728
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	AU 2003258538	A1	20040319	AU 2003-258538	20030728
	EP 1532090	A1	20050525	EP 2003-790821	20030728
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	JP 2005537334	T	20051208	JP 2004-569707	20030728
	US 2006165915	A1	20060727	US 2005-524846	20050218
PRAI	DE 2002-10238999	A	20020826		
	DE 2003-10324843	A	20030602		
	WO 2003-EP8285	W	20030728		

CLASS

	PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
	DE 10238999	ICM	C07C025-22
		ICS	C07C043-225; C07C049-697; C07D319-06; C09K019-32; C09K019-34; G02F001-137; G09F009-35; C07C069-00; C07C323-00; C07C255-00; C07C331-00
		IPCI	C07C0025-22 [ICM,7]; C07C0025-00 [ICM,7,C*]; C07C0043-225 [ICS,7]; C07C0043-00 [ICS,7,C*]; C07C0049-697 [ICS,7]; C07C0049-00 [ICS,7,C*]; C07D0319-06 [ICS,7]; C07D0319-00 [ICS,7,C*]; C09K0019-32 [ICS,7]; C09K0019-34 [ICS,7]; G02F0001-137 [ICS,7]; G02F0001-13 [ICS,7,C*]; G09F0009-35 [ICS,7]; C07C0069-00 [ICS,7]; C07C0323-00 [ICS,7]; C07C0255-00 [ICS,7]; C07C0331-00 [ICS,7]
		IPCR	C07C0017-00 [I,C*]; C07C0017-093 [I,A]; C07C0017-25 [I,A]; C07C0017-35 [I,A]; C07C0017-354 [I,A]; C07C0022-00 [I,C*]; C07C0022-08 [I,A]; C07C0025-00 [I,C*]; C07C0025-22 [I,A]; C07C0025-24 [I,A]; C07C0045-00 [I,C*]; C07C0045-46 [I,A]; C07C0045-64 [I,A]; C07C0049-00 [I,C*]; C07C0049-697 [I,A]; C07C0255-00 [I,C*]; C07C0255-52 [I,A]; C09K0019-32 [I,A]; C09K0019-32 [I,C*]; C09K0019-34 [I,A]; C09K0019-34 [I,C*]
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WO 2004020375		IPCI	C07C0025-22 [ICM,7]; C07C0022-08 [ICS,7]; C07C0022-00 [ICS,7,C*]; C07C0025-24 [ICS,7]; C07C0025-00 [ICS,7,C*]; C07C0043-225 [ICS,7]; C07C0043-00 [ICS,7,C*]; C09K0019-32 [ICS,7]
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US 2006165915	IPCI	C09K0019-32 [I,A]; C09K0019-34 [I,A]; C07C0013-54 [I,A]; C07C0013-547 [I,A]; C07C0013-00 [I,C*]
	IPCR	C09K0019-32 [I,A]; G02F0001-139 [I,A]; C07C0013-00 [I,C]; C07C0013-54 [I,A]; C07C0013-547 [I,A]; C07C0017-00 [I,C*]; C07C0017-093 [I,A]; C07C0017-25 [I,A]; C07C0017-35 [I,A]; C07C0017-354 [I,A]; C07C0022-00 [I,C*]; C07C0022-08 [I,A]; C07C0025-00 [I,C*]; C07C0025-22 [I,A]; C07C0025-24 [I,A]; C07C0045-00 [I,C*]; C07C0045-46 [I,A]; C07C0045-64 [I,A]; C07C0049-00 [I,C*]; C07C0049-697 [I,A]; C07C0255-00 [I,C*]; C07C0255-52 [I,A]; C09K0019-32 [I,C]; C09K0019-34 [I,C]; C09K0019-34 [I,A]; C09K0019-54 [I,C*]; C09K0019-54 [I,A]; G02F0001-13 [I,C*]; G02F0001-13 [I,A]
	NCL	428/001.100; 252/299.610; 252/299.620; 585/021.000
	ECLA	C07C017/093+25/22; C07C017/25+25/22; C07C017/25+25/24; C07C017/35+25/22; C07C017/35+25/24; C07C017/354+25/22;

C07C022/08; C07C025/22; C07C025/24; C07C045/46+49/697;  
C07C045/46+49/755; C07C045/64+49/747; C07C049/697;  
C07C255/52; C09K019/32; C09K019/34A



AB The title cyclopenta[b]naphthalene derivative having a neg.  $\Delta\epsilon$  is represented by general formula I, II, III, IV and V (B = five membered ring with F-substituent; A = 1,4-phenylene, etc.; Z = single bond, double bond, -CF<sub>2</sub>O-, etc.; R = H, C1-15-alkyl, alkoxy, etc.; X, L = H, C1-15-alkyl, etc.; E, G = H, C1-15-alkyl, etc.; n = 0-3). The cyclopenta[b]naphthalene derivs. are synthesized.

ST nematic liq crystal mixt display cyclopenta naphthalene prepns

IT Liquid crystal displays  
 (cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)

IT Liquid crystals  
 (nematic; cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)

IT 666732-85-0P 666732-87-2P 666732-89-4P  
 666732-91-8P 666732-93-0P 666732-95-2P 666732-97-4P  
 666732-99-6P 666733-01-3P 666733-03-5P 666733-05-7P 666733-07-9P  
 666733-09-1P 666733-11-5P 666733-13-7P  
 666733-15-9P

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
 (preparation of cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)

IT 75-77-4, Chlorotrimethylsilane, reactions 77-48-5, 1,3-Dibromo-5,5-dimethylhydantoin 100-39-0 109-80-8, 1,3-Propanedithiol 540-63-6, 1,2-Ethanedithiol 7664-39-3, Hydrogen fluoride, reactions 57848-46-1 104089-16-9 107263-95-6, N-Fluoropyridinium triflate 610312-65-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)

IT 13772-59-3P 666732-11-2P 666732-13-4P 666732-15-6P 666732-17-8P  
 666732-19-0P 666732-22-5P 666732-24-7P 666732-26-9P 666732-28-1P

666732-30-5P 666732-32-7P 666732-36-1P 666732-38-3P 666732-40-7P  
666732-42-9P 666732-44-1P 666732-46-3P 666732-48-5P 666732-50-9P  
666732-52-1P 666732-55-4P 666732-57-6P 666732-59-8P 666732-61-2P  
666732-63-4P 666732-65-6P 666732-67-8P 666732-69-0P 666732-71-4P  
666732-74-7P 666732-76-9P 666732-79-2P 666732-81-6P 666732-83-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)

IT 666732-85-0P 666732-87-2P 666732-89-4P  
666732-91-8P 666733-11-5P 666733-13-7P  
666733-15-9P

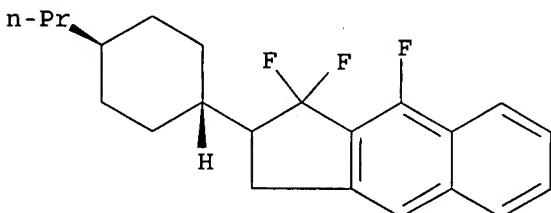
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of cyclopenta[b]naphthalene derivate useful in nematic liquid crystal mixture suitable for liquid crystal display)

RN 666732-85-0 CAPPLUS

CN 1H-Benz[f]indene, 1,1,9-trifluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

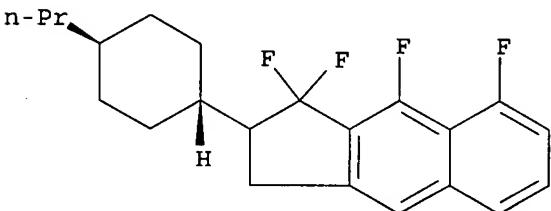
Relative stereochemistry.



RN 666732-87-2 CAPPLUS

CN 1H-Benz[f]indene, 1,1,8,9-tetrafluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

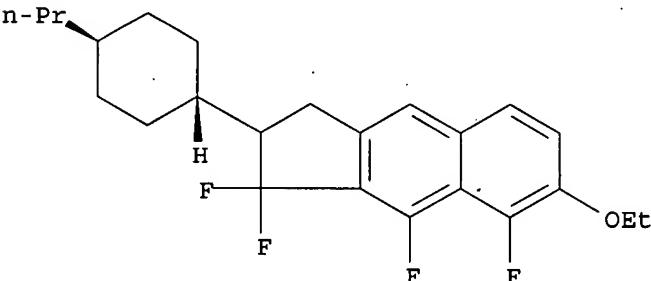
Relative stereochemistry.



RN 666732-89-4 CAPPLUS

CN 1H-Benz[f]indene, 7-ethoxy-1,1,8,9-tetrafluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

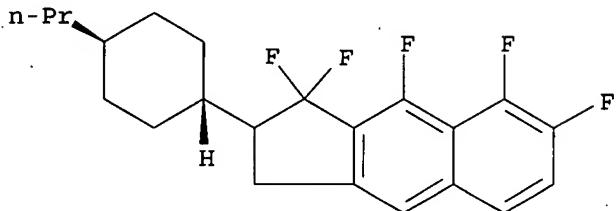
Relative stereochemistry.



RN 666732-91-8 CAPLUS

CN 1H-Benz[f]indene, 1,1,7,8,9-pentafluoro-2,3-dihydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

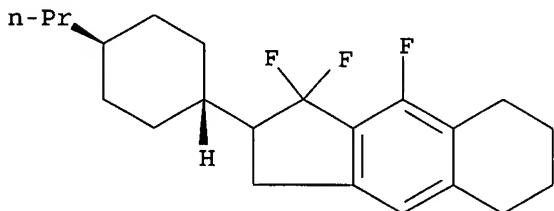
Relative stereochemistry.



RN 666733-11-5 CAPLUS

CN 1H-Benz[f]indene, 1,1,9-trifluoro-2,3,5,6,7,8-hexahydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

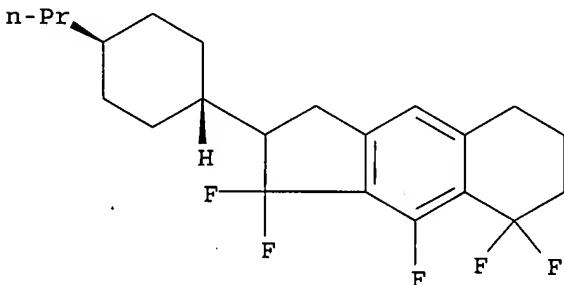
Relative stereochemistry.



RN 666733-13-7 CAPLUS

CN 1H-Benz[f]indene, 1,1,8,8,9-pentafluoro-2,3,5,6,7,8-hexahydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

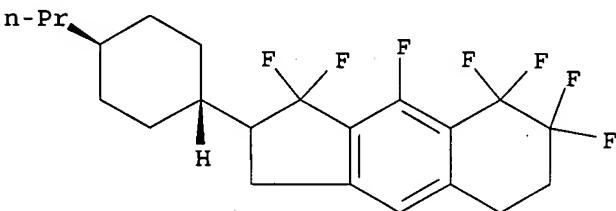
Relative stereochemistry.



RN 666733-15-9 CAPLUS

CN 1H-Benz[f]indene, 1,1,7,7,8,8,9-heptafluoro-2,3,5,6,7,8-hexahydro-2-(trans-4-propylcyclohexyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2002:817619 CAPLUS  
DN 138:237618  
ED Entered STN: 28 Oct 2002  
TI MNDO Study of the (Anti)aromaticity of Fluorine-Containing Cyclopentadienyl, Indenyl, and Cyclopenta[b]naphthyl Cations  
AU Shchegoleva, L. N.; Karpov, V. M.; Platonov, V. E.  
CS Siberian Division, Vorozhtsov Novosibirsk Institute of Organic Chemistry, Russian Academy of Sciences, Novosibirsk, 630090, Russia  
SO Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (2002), 38(7), 995-1000  
CODEN: RJOCEQ; ISSN: 1070-4280  
PB MAIK Nauka/Interperiodica Publishing  
DT Journal  
LA English  
CC 22-2 (Physical Organic Chemistry)  
AB MNDO calcns. were performed to estimate the aromaticity (antiaromaticity) of F-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations in terms of the Dewar-Breslow criterion which uses the difference in the enthalpies of formation of isomeric cations with closed and open  $\pi$ -systems as aromaticity index. The aromaticity is strongly determined by both the structure of the C skeleton and the number and position of F atoms. A linear correlation was revealed between the aromaticity index and the energy of the lowest singlet-singlet excitation for cations having a cyclic  $\pi$ -system.  
ST MNDO aromaticity antiaromaticity fluorine cyclopentadienyl indenyl cyclopantanaphthyl cation  
IT Linear free energy relationship  
(Dewar-Breslow aromaticity index vs. singlet excitation; MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)  
IT Antiaromaticity  
Aromaticity  
Correlation analysis  
Formation enthalpy  
Frontier molecular orbital  
HOMO (molecular orbital)  
Jahn-Teller effect  
LUMO (molecular orbital)  
MNDO  
Singlet state excitation  
Substituent effects  
(MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)  
IT Carbocations  
RL: PRP (Properties)  
(MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)  
IT Indexes  
(aromaticity; MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)  
IT Isomers  
(cation; MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)  
IT 49762-89-2 58741-78-9 62302-99-2 128654-07-9 192275-45-9  
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501370-93-0  
RL: PRP (Properties)  
(MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD

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- (2) Breslow, R; Acc Chem Res 1973, V6(12), P393 CAPLUS
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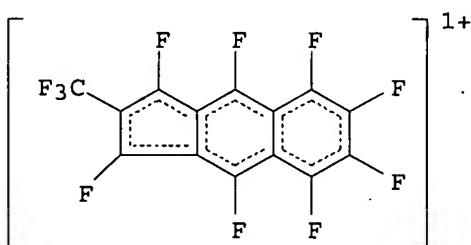
IT 501370-90-7 501370-91-8

RL: PRP (Properties)

(MNDO study of (anti)aromaticity of fluorine-containing cyclopentadienyl, indenyl, and cyclopenta[b]naphthyl cations)

RN 501370-90-7 CAPLUS

CN Benz[f]indenylum, 1,3,4,5,6,7,8,9-octafluoro-2-(trifluoromethyl)- (9CI)  
(CA INDEX NAME)



RN 501370-91-8 CAPLUS

CN Benz[f]indenylum, 1,3,4,5,8,9-hexafluoro-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

